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**Low-temperature phases of dense hydrogen and deuterium by first-principles path-integral molecular dynamics** MARC TORRENT, GREGORY GENESTE, CEA, DAM, DIF, F-91297 Arpajon, France — The low-temperature phases of dense hydrogen and deuterium have been investigated using first-principles path-integral molecular dynamics, a technique that we have recently implemented in the ABINIT code and that allows to account for the quantum fluctuations of atomic nuclei. A massively parallelized scheme is applied to produce trajectories of several tens of thousands steps using a 64-atom supercell and a Trotter number of 64. The so-called phases I, II and III are studied and compared to the structures proposed in the literature. The quantum fluctuations produce configurational disorder and are shown to systematically enhance the symmetry of the system: a continuous gain of symmetry in the angular density of probability of the molecules is found from classical particles to quantum D2 and finally to quantum H2. Particular emphasis is made on the "broken-symmetry" phase (phase II).

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